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Ground-state properties of a one-dimensional strongly interacting Bose-Fermi mixture in a double-well potential

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We calculate the reduced single-particle density matrix (RSPDM), momentum distribution, natural orbitals and their occupancies, for a strongly repulsive one-dimensional Bose-Fermi mixture in a double-well potential with a large central barrier. We assume that all particles have the same mass, and fermions are spin polarized. For mesoscopic systems, we find that the ground-state properties qualitatively differ for mixtures with even number of particles (both odd-odd and even-even mixtures) in comparison to mixtures with odd particle numbers (odd-even and even-odd mixtures). For even mixtures the momentum distribution is smooth, whereas the momentum distribution of odd mixtures possesses distinct modulations; the differences are observed also in the off-diagonal correlations of the RSPDM, and in the occupancies of natural orbitals. The calculation is based on a formula which enables efficient calculation of the RSPDM for mesoscopic mixtures in various potentials.

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I. INTRODUCTION

The experiments with interacting ultracold atomic gases loaded in various external potentials offer great opportunities for probing versatile many-body states (e.g., see [1] for a review), from weakly interacting gases up to strongly correlated states. Interactions between the atoms can be tuned in some cases (e.g., by employing Feshbach resonances), while external potentials can assume various shapes including optical lattices, elongated and transversely tight traps and many others. Systems of interacting atoms in double-well potentials exhibit particularly interesting phenomena which were studied over the years, for example, a bosonic Josephson junction [2–5], squeezing and entanglement of matter waves [6,7], matter wave interference [8,9], and recently exact many-body quantum dynamics in a one-dimensional (1D) quantum well [10]. In this work we focus on a strongly repulsive Bose-Fermi mixture of particles in a 1D double well potential.

The achievement of quantum degeneracy in Bose-Fermi mixtures [11–18] has stimulated many studies of these systems. In 1D geometry, several theoretical approaches explored such mixtures. For example, the mean-field approximation has been utilized to study phase separation [19]. However, for strongly correlated systems, which are more likely to occur in one-dimensional than in three-dimensional systems, the mean field approach is not appropriate. These systems can be studied by using exactly solvable models and/or sophisticated numerical calculations. Luttinger liquid theory has been used to study pairing instabilities and phase diagrams [20,21]; (the Luttinger liquid theory can describe the low-energy properties of these systems) [20,21]. Numerical calculations were used to obtain the phase diagram for mixture with unequal masses [22]. One-dimensional Bose-Fermi mixture with a finite coupling strength and without an external trapping potential were studied in Refs. [23–25]. Recently, an exactly solvable model describing 1D Bose-Fermi mixtures with strong interactions has been studied in Ref. [26]. The ground-state wave functions for arbitrary external potentials were constructed; in the model, strong ("impenetrable core") interactions are present between bosons, bosons and fermions, whereas fermions are mutually noninteracting and they are spin polarized. The correlation functions including the one-body density matrix were addressed for the ring geometry and the harmonic confinement [26]. The ground-state properties and expansion dynamics were further explored in Ref. [27].

The solution of the model presented in Ref. [26] follows the Fermi-Bose mapping idea to calculate exact wave functions in the so called Tonks-Girardeau (TG) model of "impenetrable-core" bosons [28]. This model has been experimentally realized several years ago [29,30], with atoms in tight transversely confined atomic waveguides [31], at low temperatures, and with strong effective interactions [31–33]. Besides the wave functions [28], the correlation functions such as the reduced single-particle density matrix (RSPDM) and related quantities including distributions of momenta, natural orbitals and their occupancies, have been studied for the TG system over the years [34–45] for the ground states on the circle [34,38], in harmonic confinement [36–39], for excited "dark-soliton" eigenstates [43], in a split-trap potential [44,45], and also for time-dependent states (e.g., see [40–42]).

Here we study ground-state properties of a strongly repulsive Bose-Fermi mixture in a double-well potential; we use the model from Ref. [26] where all particles are assumed to have the same mass, and fermions are spin polarized. As a first step, we derive a formula which enables efficient calculation of the RSPDM for mesoscopic mixtures in various

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potentials; it reduces to a calculation of RSPDM for TG bosons [42] in an incoherent mixed state. The formula is employed to calculate the RSPDM, momentum distribution, natural orbitals and their occupancies, for the ground state of a mixture in a double well. For mesoscopic systems, we find that the ground state properties qualitatively differ for mixtures with even number of particles (both odd-odd and even-even mixtures) in comparison to mixtures with odd particle numbers (odd-even and even-odd mixtures). For even mixtures the momentum distribution is smooth, whereas the momentum distribution of odd mixtures possesses modulations; the differences are observed also in the off-diagonal correlations of the RSPDM, and in the occupancies of natural orbitals.

II. MODEL

We study a mixture of N_B bosons and N_F spin-polarized fermions in one-dimensional geometry, in a ground state of an external potential $V(x)$. Bosons and fermions experience the same external potential, and their masses are assumed to be approximately equal. This condition can be satisfied for combination of bosonic and fermionic isotopes of the same element, such as $^{39(41)}$K-^{40}K, or Yb with several stable isotopes, and $^{86(84)}$Rb-$^{87(85)}$Rb (for detailed discussion, see [23] and references therein). Bosons interact via a very strong repulsive contact potential, that is, their interaction is in the Tonks-Girardeau regime. Fermions are mutually noninteracting. Interaction between bosons and fermions is also a very strong repulsive contact potential. The total number of particles is denoted with $N=N_B+N_F$. The resulting Hamiltonian reads

$$\hat{H}=\hat{H}_B+\hat{H}_F+\hat{H}_{BB}+\hat{H}_{BF}, \tag{1}$$

where

$$\hat{H}_B=\sum_{j=1}^{N_B}\left[-\frac{\partial^2}{\partial x_{Bj}^2}+V(x_{Bj})\right],$$

$$\hat{H}_F=\sum_{j=1}^{N_F}\left[-\frac{\partial^2}{\partial x_{Fj}^2}+V(x_{Fj})\right],$$

$$\hat{H}_{BB}=\sum_{1\le i<j\le N_B} g_{BB}\delta(x_{Bj}-x_{Bi}),$$

$$\hat{H}_{BF}=\sum_{j=1}^{N_B}\sum_{i=1}^{N_F} g_{BF}\delta(x_{Bj}-x_{Fi}),$$

with $V(x)$ being some external potential and g_{BB} and g_{BF} are the coupling constants.

The ground state for this system for finite but very strong repulsive interactions (i.e., g_{BB} and g_{BF} are sufficiently large to be approximately treated as if they are infinite) can be approximately written as [26]

$$\begin{aligned}\psi(x_{F1},\ldots,x_{FN_F},x_{B1},\ldots,x_{BN_B}) &= \prod_{1\le i<j\le N_B}\operatorname{sgn}(x_{Bj}-x_{Bi})\prod_{j=1}^{N_B}\prod_{i=1}^{N_F}\operatorname{sgn}(x_{Bj}-x_{Fi})\\ &\quad\times\psi_S(x_{F1},\ldots,x_{FN_F},x_{B1},\ldots,x_{BN_B}).\end{aligned} \tag{2}$$

Here,

$$\psi_S(x_1,\ldots,x_N)=\frac{1}{\sqrt{N!}}\sum_{P\in S_N}(-)^P\phi_{Pj_1}(x_1)\ldots\phi_{Pj_N}(x_N), \tag{3}$$

denotes a Slater determinant wave function constructed from the single-particle wave functions $\phi_j(x)$, which are the N lowest single-particle eigenstates of the potential $V(x)$,

$$-\frac{d^2\phi_j(x)}{dx^2}+V(x)\phi_j(x)=E_j\phi_j(x), \tag{4}$$

$j=1,2,\ldots,N=N_F+N_B$. In Eq. (3), P denotes a permutation from the group S_N. For the clarity of the exposition, it is convenient to define the following quantities. Let us consider a subset of single-particle states, chosen from the set $\{\phi_j(x)|j=1,\ldots,N\}$ by crossing out k single-particle states; let $J=\{j_1,j_2,\ldots,j_k\}$ denote the indices of the crossed states, and $L=\{l_1,l_2,\ldots,l_{N-k}\}$ the indices of the remaining states (obviously $J\cap L=\emptyset$, $J\cup L=\{1,\ldots,N\}$). We define the Slater determinant state

$$\psi_S^{(j_1,j_2,\ldots,j_k)}(x_1,\ldots,x_{N-k}) = \frac{1}{\sqrt{(N-k)!}}\sum_{P\in S_{N-k}}(-)^P\phi_{Pl_1}(x_1)\ldots\phi_{Pl_{N-k}}(x_{N-k}), \tag{5}$$

where P is a permutation of indices $(l_1,l_2,\ldots,l_{N-k})$. Thus, the indices upon $\psi_S^{(j_1,j_2,\ldots,j_k)}$ denote the crossed out states, rather than the ones used in the Slater determinant.

Let $\psi_{TG}^{(j_1,j_2,\ldots,j_k)}=A\psi_S^{(j_1,j_2,\ldots,j_k)}$ denote a symmetric Tonks-Girardeau state obtained by acting with a unit antisymmetric function $A=\prod_{1\le i<j\le N-k}\operatorname{sgn}(x_j-x_i)$ upon $\psi_S^{(j_1,j_2,\ldots,j_k)}$. The RSPDM of the state $\psi_{TG}^{(j_1,j_2,\ldots,j_k)}$ will be denoted by $\rho_{TG}^{(j_1,j_2,\ldots,j_k)}$,

$$\begin{aligned}\rho_{TG}^{(j_1,j_2,\ldots,j_k)}(x,y) &= (N-k)\int dx_2\ldots dx_{N-k}\\ &\quad\times\psi_{TG}^{(j_1,j_2,\ldots,j_k)}(x,x_2\ldots,x_{N-k})^*\\ &\quad\times\psi_{TG}^{(j_1,j_2,\ldots,j_k)}(y,x_2\ldots,x_{N-k}).\end{aligned} \tag{6}$$

The quantities ψ_S, ψ_{TG}, and ρ_{TG} etc. will refer to states and the correlation functions obtained from the full set of single-particle states $\{\phi_j(x)|j=1,\ldots,N\}$.

III. FORMULA FOR THE RSPDM

We are interested in properties of the ground state of the Bose-Fermi mixture described by the state (2). To explore the one-particle observables of this Bose-Fermi mixture, we need to construct the RSPDM of the bosonic and the fermionic subsystems, respectively. The one-body density matrix for the bosonic part of the mixture is defined as

$$\eta_{N_B,N_F}(x,y) = N_B \int dx_{F1} \dots dx_{FN_F} dx_{B2} \dots dx_{BN_B} \times \psi^*(x_{F1}, \dots, x_{FN_F}, x, x_{B2}, \dots, x_{BN_B}) \times \psi(x_{F1}, \dots, x_{FN_F}, y, x_{B2}, \dots, x_{BN_B}). \quad (7)$$

It is straightforward to verify that $\eta_{N_B,N_F}(x,y)$ can be calculated from the RSPDM describing N Tonks-Girardeau bosons, $\eta_{N_B,N_F}(x,y)=N_B/N\rho_{TG}(x,y)$. This correlation function can be efficiently calculated by using the procedure derived in Ref. [42] (the procedure was recently also generalized to describe hard-core anyonic gases [46]).

The calculation of the density matrix describing the fermionic component of the mixture,

$$\mu_{N_B,N_F}(x,y) = N_F \int dx_{F2} \dots dx_{FN_F} dx_{B1} \dots dx_{BN_B} \times \psi^*(x, x_{F2}, \dots, x_{FN_F}, x_{B1}, \dots, x_{BN_B}) \times \psi(y, x_{F2}, \dots, x_{FN_F}, x_{B1}, \dots, x_{BN_B}), \quad (8)$$

is much more involved. The derivation can be reduced to calculations of the RSPDM for an incoherent mixed TG state as follows:

$$\mu_{N_B,N_F}(x,y) = \frac{N_F}{N!} \int dx_{F2} \dots dx_{FN_F} dx_{B1} \dots dx_{BN_B} \times \prod_{i=1}^{N_B} \mathrm{sgn}(x-x_{Bi})\mathrm{sgn}(y-x_{Bi}) \times \begin{vmatrix} \phi_1^*(x) & \dots & \phi_N^*(x) \\ \phi_1^*(x_{F2}) & \dots & \phi_N^*(x_{F2}) \\ \vdots & \ddots & \vdots \\ \phi_1^*(x_{FN_F}) & \dots & \phi_N^*(x_{FN_F}) \\ \phi_1^*(x_{B1}) & \dots & \phi_N^*(x_{B1}) \\ \vdots & \ddots & \vdots \\ \phi_1^*(x_{BN_B}) & \dots & \phi_N^*(x_{BN_B}) \end{vmatrix} \times \begin{vmatrix} \phi_1(y) & \dots & \phi_N(y) \\ \phi_1(x_{F2}) & \dots & \phi_N(x_{F2}) \\ \vdots & \ddots & \vdots \\ \phi_1(x_{FN_F}) & \dots & \phi_N(x_{FN_F}) \\ \phi_1(x_{B1}) & \dots & \phi_N(x_{B1}) \\ \vdots & \ddots & \vdots \\ \phi_1(x_{BN_B}) & \dots & \phi_N(x_{BN_B}) \end{vmatrix}. \quad (9)$$

The determinants above can be expanded along their second row according to the Laplace formula, after which the integral over x_{F2} is trivially performed,

$$\mu_{N_B,N_F}(x,y) = \frac{N_F}{N!} \int dx_{F3} \dots dx_{FN_F} dx_{B1} \dots dx_{BN_B} \prod_{i=1}^{N_B} \mathrm{sgn}(x-x_{Bi})\mathrm{sgn}(y-x_{Bi}) \sum_{j,l=1}^{N} (-)^{2+j}(-)^{2+l} \int \phi_j^*(x_{F2})\phi_l(x_{F2})dx_{F2}$$
$$\times \begin{vmatrix} \phi_1^*(x) & \cdots & \phi_{j-1}^*(x) & \phi_{j+1}^*(x) & \cdots & \phi_N^*(x) \\ \phi_1^*(x_{F3}) & \cdots & \phi_{j-1}^*(x_{F3}) & \phi_{j+1}^*(x_{F3}) & \cdots & \phi_N^*(x_{F3}) \\ \vdots & & \vdots & \vdots & & \vdots \\ \phi_1^*(x_{FN_F}) & \cdots & \phi_{j-1}^*(x_{FN_F}) & \phi_{j+1}^*(x_{FN_F}) & \cdots & \phi_N^*(x_{FN_F}) \\ \phi_1^*(x_{B1}) & \cdots & \phi_{j-1}^*(x_{B1}) & \phi_{j+1}^*(x_{B1}) & \cdots & \phi_N^*(x_{B1}) \\ \vdots & & \vdots & \vdots & & \vdots \\ \phi_1^*(x_{BN_B}) & \cdots & \phi_{j-1}^*(x_{BN_B}) & \phi_{j+1}^*(x_{BN_B}) & \cdots & \phi_N^*(x_{BN_B}) \end{vmatrix}$$
$$\times \begin{vmatrix} \phi_1(y) & \cdots & \phi_{l-1}(y) & \phi_{l+1}(y) & \cdots & \phi_N(y) \\ \phi_1(x_{F3}) & \cdots & \phi_{l-1}(x_{F3}) & \phi_{l+1}(x_{F3}) & \cdots & \phi_N(x_{F3}) \\ \vdots & & \vdots & \vdots & & \vdots \\ \phi_1(x_{FN_F}) & \cdots & \phi_{l-1}(x_{FN_F}) & \phi_{l+1}(x_{FN_F}) & \cdots & \phi_N(x_{FN_F}) \\ \phi_1(x_{B1}) & \cdots & \phi_{l-1}(x_{B1}) & \phi_{l+1}(x_{B1}) & \cdots & \phi_N(x_{B1}) \\ \vdots & & \vdots & \vdots & & \vdots \\ \phi_1(x_{BN_B}) & \cdots & \phi_{l-1}(x_{BN_B}) & \phi_{l+1}(x_{BN_B}) & \cdots & \phi_N(x_{BN_B}) \end{vmatrix}$$
$$= \frac{N_F}{N(N_F-1)} \sum_{j=1}^{N} \mu^{(j)}_{N_B,N_F-1}(x,y), \quad (10)$$

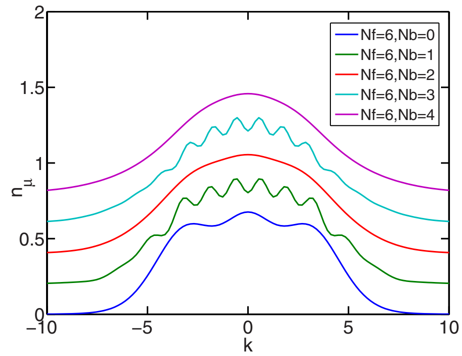

FIG. 1. (Color online) Momentum distributions $n_\mu(k)$ for $N_F=6$ (all curves) and $N_B=0,1,2,3,4$; curves are ordered from bottom to top and shifted by a constant for better visibility.

where we have used $\int \phi_j^*(x_{F2})\phi_l(x_{F2})dx_{F2}=\delta_{jl}$. The index j in $\mu^{(j)}_{N_B,N_F-1}$ means that the single-particle state ϕ_j has been crossed out from the Slater determinant used in the formula for the ground state, see Sec. II. Thus, we have derived a recursion formula which reduces the calculation of the fermionic RSPDM $\mu_{N_B,N_F}(x,y)$, to the calculation of N fermionic correlation functions, $\mu_{N_B,N_F-1}(x,y)$ (with one fermion less in the mixture). By successively applying the recursive formula above, it is straightforward to obtain

$$\mu_{N_B,N_F}(x,y) = \frac{N_F!\,(N_B+1)!}{N!} \times \sum_{1\le j_1<\ldots<j_{N_F-1}\le N} \mu^{(j_1,\ldots,j_{N_F-1})}_{N_B,1}(x,y) = \frac{N_F!\,N_B!}{N!}\sum_{1\le j_1<\ldots<j_{N_F-1}\le N}\rho^{(j_1,\ldots,j_{N_F-1})}_{TG}(x,y). \tag{11}$$

The correlation functions $\mu^{(j_1,\ldots,j_{N_F-1})}_{N_B,1}(x,y)$ correspond to a mixture with one fermion and N_B bosons; it is straightforward to see from the definition of μ_{N_B,N_F} that $\mu^{(j_1,\ldots,j_{N_F-1})}_{N_B,1}\propto\rho^{(j_1,\ldots,j_{N_F-1})}_{TG}$, i.e., the system with just one extra fermion has identical RSPDM (up to a normalization constant) to the system with N_B+1 TG bosons placed in the proper single-particle orbitals.

Thus, the density matrix $\mu_{N_B,N_F}(x,y)$ is equal (up to a proportionality constant) to a sum of density matrices of TG states from an ensemble. Each TG state from the ensemble describes N_B+1 TG bosons; these states are constructed by choosing N_B+1 orbitals from the full set of single-particle states $\{\phi_j(x)\,|\,j=1,\ldots,N\}$. Apparently, there are $\binom{N}{N_B+1}$ such states, i.e., there are $\binom{N}{N_B+1}$ terms in the sum (11). Thus, the density matrix $\mu_{N_B,N_F}(x,y)$ is equivalent to the density matrix of N_B+1 bosons in a mixed TG state; the mixed state is an incoherent superposition of the ground state and many excited TG states, each of which is constructed by some choice of N_B+1 orbitals as stated above. The calculation thus reduces to applying the algorithm of Ref. [42]. Numerical calculations become too time consuming if the number of terms in the sum (11) is too large. Nevertheless, it can be performed efficiently for mesoscopic systems.

From the RSPDM, one can extract observables such as the momentum distribution, and important quantities such as the natural orbitals (NOs) and their occupancies. For example, the fermionic momentum distribution is given by

$$n_\mu(k) = \frac{1}{2\pi}\int dxdy e^{ik(x-y)}\mu_{N_B,N_F}(x,y); \tag{12}$$

the eigenfunctions of the fermionic RSPDM, $\Phi_{\mu,i}(x)$, are called the NOs,

$$\int dx \mu_{N_B,N_F}(x,y)\Phi_{\mu,i}(x) = \lambda_{\mu,i}\Phi_{\mu,i}(y), \quad i=1,2,\ldots; \tag{13}$$

the eigenvalues $\lambda_{\mu,i}$ are the occupancies of these orbitals. The bosonic momentum distribution $n_\eta(k)$, NOs $\Phi_{\eta,i}(x)$, and occupancies $\lambda_{\eta,i}$, are defined by using equivalent relations for the bosonic RSPDM.

IV. MIXTURE IN A SPLIT TRAP

In this section we apply the presented formalism to study the RSPDM, momentum distribution, natural orbitals and their occupancies for a Bose-Fermi mixture in a double well potential of the form

$$V(x) = V_{ho}(x) + V_G(x) = \nu^2x^2 + V_0 e^{-(x/\sigma)^2}, \tag{14}$$

where the parameter σ (V_0) denotes the width (height, respectively) of the Gaussian barrier which splits the harmonic potential. We note in passing that the presented result may depend on the shape of the double-well potential (e.g., for the split-box potential) as will be discussed below. Here we work in dimensionless units; the connection to physical units can be made straightforwardly: for example, if m is the mass of bosons (which is equal to the mass of fermions), and x_{unit} the unit of space (which can be chosen at will), then the unit of energy is $E_{unit}=\hbar^2/(2mx^2_{unit})$. The single-particle eigenstates of the potential $V(x)$ are calculated numerically by employing a simple and standard scheme: the x space is dis-

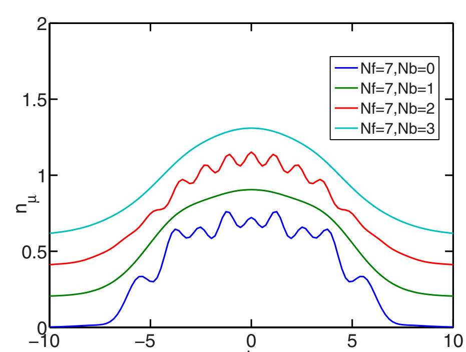

FIG. 2. (Color online) Momentum distributions $n_\mu(k)$ for $N_F=7$ (all curves) and $N_B=0,1,2,3$: curves are ordered from bottom to top and shifted by a constant for better visibility.

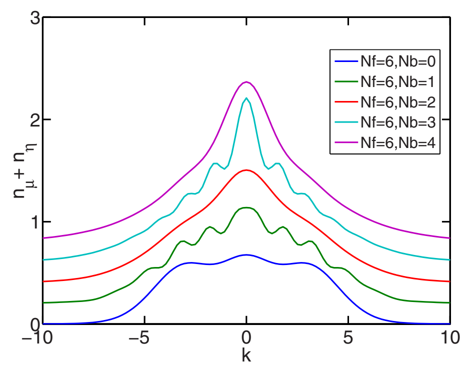

FIG. 3. (Color online) The total momentum distributions $n_\mu(k)+n_\eta(k)$ for $N_F=6$ (all curves) and $N_B=0,1,2,3,4$; curves are ordered from bottom to top and shifted by a constant for better visibility.

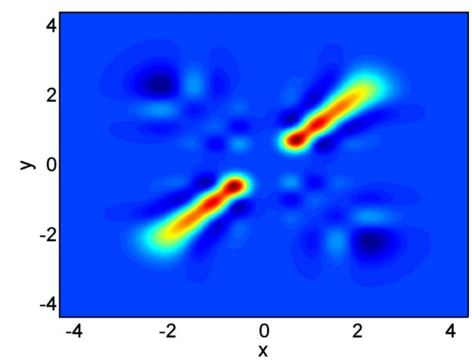

FIG. 5. (Color online) Contour plot of the fermionic RSPDM for $N_F=6$ and $N_B=1$.

cretized in 1024 equidistant points, the second-derivative operator is represented in a simple tridiagonal matrix form, and finally the single-particle eigenstates are found by diagonalizing the tridiagonal matrix which represents the single-particle Hamiltonian.

In what follows we present results of numerical simulations for the double-well parameters $\sigma=0.3$ and $V_0=230$; the harmonic trap frequency parameter is $\nu^2=7.5$. It should be emphasized that we have focused our attention to the cases when the splitting potential is sufficiently high, say, when V_0 is at least several times larger than the energy of the Nth single-particle state of the potential $V_{ho}(x)$. Thus, all our conclusions should be understood to hold in this limit. The momentum distribution of the bosonic component was shown to be equivalent to that of N TG bosons placed within $V(x)$ and this case has already been addressed in Ref. [44]. Thus, we first turn our attention to the behavior of the fermionic momentum distribution in the mixture $n_\mu(k)$, as a function of the number of particles. Figure 1 shows $n_\mu(k)$ for $N_F=6$ and $N_B=0,1,2,3,4$, while Fig. 2 shows the same quantity for $N_F=7$ and $N_B=0,1,2,3$. From these figures we observe a qualitative difference in behavior of the fermionic momentum distribution in dependence on the parity of the total number of particles $N=N_F+N_B$: if N is even, then $n_\mu(k)$ has a smooth bell-shaped profile. In contrast, when N is odd, then there are non-negligible modulations on top of the bell-shaped profile of $n_\mu(k)$; in our simulations, for the parameters presented here, we find that the number of peaks in $n_\mu(k)$ for odd N is the same as the number of fermions in the mixture N_F plus two additional humps on the side bands of the distribution. This parity dependent behavior is reflected onto the behavior of the total momentum distributions $[n_\mu(k)+n_\eta(k)]$ which are displayed in Figs. 3 and 4 for the same combinations of particles as presented in Figs. 1 and 2. Interestingly, odd-odd combinations yield results very similar to the even-even ones, whereas even-odd combination yields results similar to the odd-even combinations. Thus, the parity of the *total* number of particles determines the behavior of the fermionic component, at least for the mesoscopic numbers of particles studied here.

The behavior of the fermionic momentum distribution results from the properties of the fermionic density matrix $\mu_{N_B,N_F}(x,y)$ which is illustrated in Fig. 5 for $N_F=6$ and $N_B=1$, Fig. 6 for $N_F=6$ and $N_B=2$, Fig. 7 for $N_F=7$ and $N_B=1$, and in Fig. 8 for $N_F=7$ and $N_B=2$. From these figures we observe that the most significant difference between the total even and odd numbers of particles occurs in the second and the fourth quadrant of the x-y plane: if N is even, the values of the fermionic RSPDM for $x<0<y$ and $y<0<x$ are negligible, $\mu_{N_B,N_F}(x,y)\approx 0$. In contrast to that, if N is odd, there are some oscillations of RSPDM in the second and the fourth quadrant, in particular close to the line $\mu_{N_B,N_F}(x,-x)$. These observations indicate that there is much greater spatial coherence between the fields at the two sides

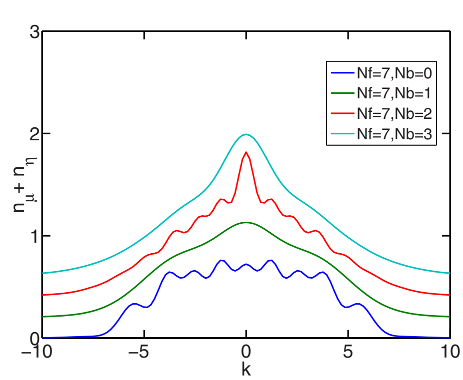

FIG. 4. (Color online) The total momentum distributions $n_\mu(k)+n_\eta(k)$ for $N_F=7$ (all curves) and $N_B=0,1,2,3$; curves are ordered from bottom to top and shifted by a constant amount for better visibility.

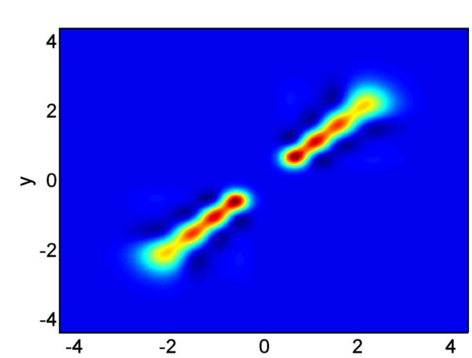

FIG. 6. (Color online) Contour plot of the fermionic RSPDM for $N_F=6$ and $N_B=2$.

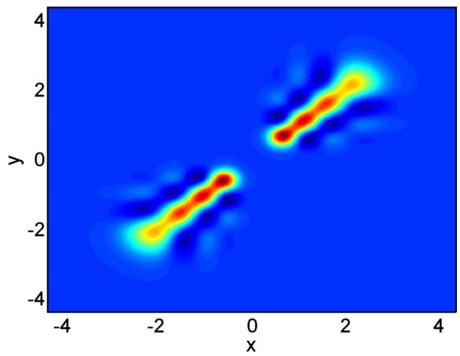

FIG. 7. (Color online) Contour plot of the fermionic RSPDM for $N_F=7$ and $N_B=1$.

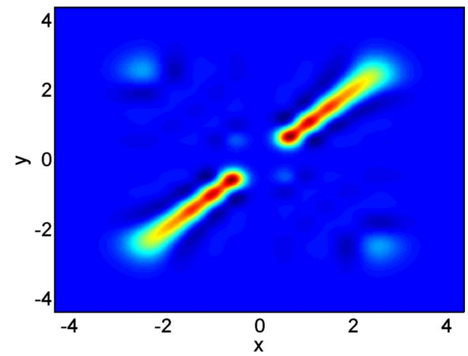

FIG. 8. (Color online) Contour plot of the fermionic RSPDM for $N_F=7$ and $N_B=2$.

of the well for odd N. A similar observation has been made for the TG gas in a split trap [44].

Let us now focus on the natural orbitals, that is, their occupancies. The occupancies $\lambda_{\mu,i}$ corresponding to the four fermionic density matrices from Figs. 5–8 are illustrated in Figs. 9 and 10. We immediately observe that when the total number of particles is even, the occupancies come in pairs and they correspond to the degenerate natural orbitals. Namely, for the total even numbers of particles the symmetry of the system with respect to the double well is naturally preserved. However, for the total odd number of particles this is not the case, which is reflected in the occupancies which do not come in degenerate pairs but rather decrease one by one.

The observation on the off-diagonal behavior of the fermionic RSPDM can be underpinned analytically. To this end, let us assume that the trap is split by an infinitely strong delta function, i.e., the mixture is in the potential $V(x)=V_{\text{trap}}+\kappa\delta(x)$, where $\kappa\to\infty$; the potential V_{trap} can be a harmonic oscillator trap, or it may have some other functional form. For the strongly repulsive Bose-Fermi mixture in a ground state of such a potential we can prove the following: if the total number of particles N is even, then $\mu_{N_B,N_F}(x,y)=0$ in the second and the fourth quadrant of the x-y plane, that is, for $x<0<y$ and $x>0>y$.

Consecutive single-particle states in a split-trap potential are degenerate, i.e., $E_{2m-1}=E_{2m}$ for $m=1,2,\ldots$; moreover, degenerate eigenstates are simply related: $\phi_{2m}(x)=\text{sgn}(x)\phi_{2m-1}(x)$. By using this relation, one of the two Slater determinants [Eq. (3)] which enter the formula for the RSPDM [Eq. (8)] [the determinant which depends on variable x] can be written as

$$\psi_S=\begin{pmatrix} \phi_1(x) & \text{sgn}(x)\phi_1(x) & \cdots & \phi_{N-1}(x) & \text{sgn}(x)\phi_{N-1}(x) \\ \phi_1(x_2) & \text{sgn}(x_2)\phi_1(x_2) & \cdots & \phi_{N-1}(x_2) & \text{sgn}(x_2)\phi_{N-1}(x_2) \\ \vdots & \vdots & & \vdots & \vdots \\ \phi_1(x_N) & \text{sgn}(x_N)\phi_1(x_N) & \cdots & \phi_{N-1}(x_N) & \text{sgn}(x_N)\phi_{N-1}(x_N) \end{pmatrix}. \tag{15}$$

Here we have simplified the notation and labeled the coordinates as x_j, where j runs up to the total number of particles N, that is, we do not explicitly refer to the fermionic or bosonic coordinates, as it is redundant for the proof. Let us assume that $x<0<y$, and that N_1 coordinates are negative, N_2 are positive, $N_1>N_2$, and $N_1+N_2=N$. First, let us demonstrate that the determinant (15) is zero in this case. In order to see that, we assume that $x,x_2,\ldots,x_{N_1}<0$, and that the rest of the coordinates are positive (due to the antisymmetry of the Slater determinant, any other choice of positive and negative coordinates would yield the same result). Let us add the first column to the second one in Eq. (15), then the third to the fourth column and so on to obtain

$$\psi_S=\begin{pmatrix} \phi_1(x) & 0 & \cdots & \phi_{N-1}(x) & 0 \\ \phi_1(x_2) & 0 & \cdots & \phi_{N-1}(x_2) & 0 \\ \vdots & \vdots & & \vdots & \vdots \\ \phi_1(x_{N_1}) & 0 & \cdots & \phi_{N-1}(x_{N_1}) & 0 \\ \phi_1(x_{N_1+1}) & 2\phi_1(x_{N_1+1}) & \cdots & \phi_{N-1}(x_{N_1+1}) & 2\phi_N(x_{N_1+1}) \\ \vdots & \vdots & & \vdots & \vdots \\ \phi_1(x_N) & 2\phi_1(x_N) & \cdots & \phi_{N-1}(x_N) & 2\phi_{N-1}(x_N) \end{pmatrix}. \tag{16}$$

Thus, the first N_1 entries of every even column, $2,4,\ldots,N$, is zero. Suppose that we shift all these even columns all the way to the right; the determinant is then proportional to

$$\begin{pmatrix} \phi_1(x) & \phi_3(x) & \cdots & \phi_{N-1}(x) & 0 & \cdots & 0 \\ \phi_1(x_2) & \phi_3(x_2) & \cdots & \phi_{N-1}(x_2) & 0 & \vdots & 0 \\ \vdots & \vdots & & \vdots & \vdots & & \vdots \\ \phi_1(x_{N_1}) & \phi_3(x_{N_1}) & \cdots & \phi_{N-1}(x_{N_1}) & 0 & \cdots & 0 \\ \phi_1(x_{N_1+1}) & \phi_3(x_{N_1+1}) & \cdots & \phi_{N-1}(x_{N_1+1}) & 2\phi_1(x_{N_1+1}) & \cdots & 2\phi_{N-1}(x_{N_1+1}) \\ \vdots & \vdots & & \vdots & \vdots & & \vdots \\ \phi_1(x_N) & \phi_3(x_N) & \cdots & \phi_{N-1}(x_N) & 2\phi_1(x_N) & \cdots & 2\phi_{N-1}(x_N) \end{pmatrix}. \tag{17}$$

In the upper right corner there is a block of zeros with the size $N_1 \times N/2$. Since $N_1 > N/2$, the determinant is identically zero. In fact, it is straightforward to verify by using the procedure outlined above that the determinant is exactly zero whenever $N_1 \neq N_2$. On the other hand, if $N_1 = N_2$, then the other Slater determinant entering the formula for the RSPDM in Eq. (8) [the one which depends on y variable], does not have equal number of positive and negative coordinates and therefore it is zero, which completes our proof. It is straightforward to see that the same result holds for the bosonic part of the mixture, and therefore for the mixture as a whole. This result can be interpreted as follows: if two slits were opened on the opposite sides of the barrier, and if the gas was allowed to drop from the slits, expand, and interfere, the interference fringes would have not been observed for even N and sufficiently high barrier. In fact, such an experiment could (at least in principle) be used to determine the parity of the mixture.

The differences in the reduced one-body density matrix and consequently in the momentum distribution between even and odd numbers of particles in the split harmonic trap can be explained as follows. Due to the fact that masses of the bosons and fermions are assumed to be identical, and because the interactions are strongly repulsive (which means that the wave function vanishes whenever any two of the particles touch), the effects of the interactions and statistics are hard to distinguish in such a one-dimensional system [26,27] (see also a study on fermionization in 1D Bose-Bose mixtures [47]). For example, the probability density is identical for the Bose-Fermi mixture considered here, for N TG bosons, or N noninteracting fermions; it is given by the Slater determinant constructed from the N lowest single-particle eigenstates. These single-particle states come in nearly degenerate pairs of even and odd eigenstates (the barrier is high, but still of finite height); thus, in order to construct the ground state, one can approximately utilize the superposition of these eigenstates, $1/\sqrt{2}(\phi_{\text{even}} \pm \phi_{\text{odd}})$, which are nearly zero either in the left, or in the right well. Consider a case where N is even. When a pair of particles is placed in a split trap, one particle of the pair is placed to the left side, and the other particle on the right side (in terms of the probability density). This means that in the ground state for even N, half of the particles are in the left, and the other half are in the right well [which corresponds to the analytical results presented in Eqs. (15)–(17)]. On the other hand, if the number of particles N is odd, the last particle cannot be placed in the left or the right well, because the Nth single-particle state is unpaired; it extends through both sides of the well and introduces correlations between the two sides of the well which we observe in the RSPDM for both fermions and bosons.

We note that this result corresponds to the observation made in Ref. [44] on the difference in spatial coherence of the Tonks-Girardeau gas in a split trap in dependence of the parity of the number of TG bosons. Our proof covers this case as well.

Finally, it is worthy to note that the shape of the external potential can influence the presented results. For example, for a box potential with a Gaussian as a split-barrier we did not find the differences between the even and odd numbers

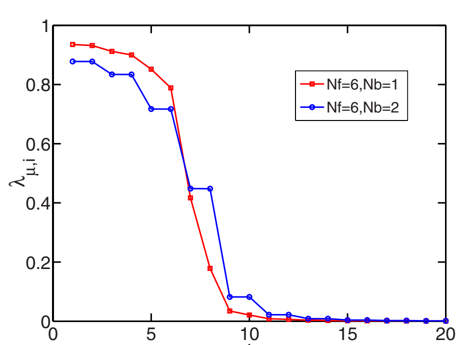

FIG. 9. (Color online) The occupancies of the fermionic RSPDM for the combinations $N_F=6$ and $N_B=1$ (squares), and $N_F=6$ and $N_B=2$ (circles). The lines serve to guide the eyes.

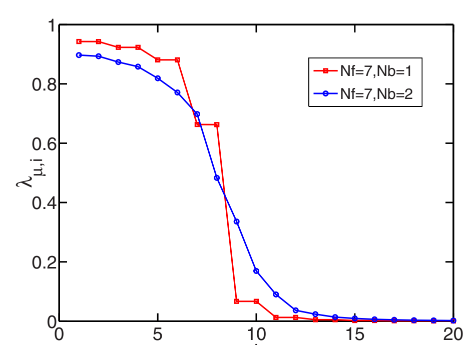

FIG. 10. (Color online) The occupancies of the fermionic RSPDM for the combinations $N_F=7$ and $N_B=1$ (squares), and $N_F=7$ and $N_B=2$ (circles). The lines serve to guide the eyes.

of particles presented above; in all cases the momentum distribution was smooth, but the differences in the RSPDM between the even and odd N were still present. For a potential of the form $\propto |x|$ with a splitting Gaussian term the differences between the odd and even numbers are recovered.

V. CONCLUSION

In conclusion, we have studied a 1D Bose-Fermi mixture, where the boson-boson and boson-fermion interactions are very strong and repulsive, whereas (spin-polarized) fermions are mutually noninteracting; the atoms in each species have approximately the same mass. The ground state for this system for finite but very strong interactions in an external potential has been constructed in Ref. [26]. We have studied the ground state properties of the mixture in a double-well trap, with a sufficiently high barrier. More specifically, a formula for the calculation of the reduced one-body density matrix of the fermionic (and also bosonic) component has been derived, which was subsequently employed to study the momentum distribution, natural orbitals and their occupancies. We have found that the behavior of the momentum distribution depends on the parity of the total number of particles: for even mixtures the momentum distribution is smooth, whereas the momentum distribution of odd mixtures possesses distinct modulations. When the total number of particles is even, the correlations expressed by the reduced one-body density matrix are negligible between the two wells.

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